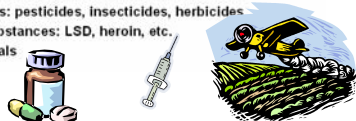


LC-MS Library Development and Strategy for Identifying Harmful Organics in Drinking Water

Lawrence Zintek, Dennis Wesolowski, Joshua Neukom – US EPA Region 5 Central Regional Laboratory
Jim Krol – Waters Corporation; Milford, MA

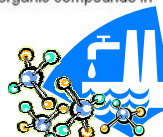
Rationale

- Developing a screening method for drinking water using LC-MS and LC-MS/MS technologies with searchable, transferable spectral libraries
- Screening method will identify harmful organic compounds not amenable to GC-MS
- Compounds amenable to LC-MS include:
 - Agrochemicals: pesticides, insecticides, herbicides
 - Controlled substances: LSD, heroin, etc.
 - Pharmaceuticals



Collaborative Science

- USEPA Region 5 Central Regional Laboratory (CRL) and Waters Corporation have formed a Cooperative Research and Development Agreement (CRADA) to build a LC-MS Library System.
- Currently, no transferable LC-MS libraries exist but GC-MS libraries (e.g. Wiley, NIST...) are in widespread use.
- This Library System would provide laboratories with a tool to tentatively identify selected harmful organic compounds in drinking water.



Instrumentation

- HPLC**
 - Waters® Alliance® 2695 HPLC unit
 - Columns
 - Atlantis® dC₁₈ 2.1 X 150mm
 - Symmetry® C₁₈ 2.1 X 150mm
 - XTerra® MS C₁₈ 2.1 X 100mm
 - Gradient: 32 min long
 - Flow Rate: 0.300 mL/min
- MS and MS/MS**
 - Micromass® Quattro micro™ API mass spectrometer
 - Software
 - MassLynx™ version 4.0 SP4



LC-MS Library System

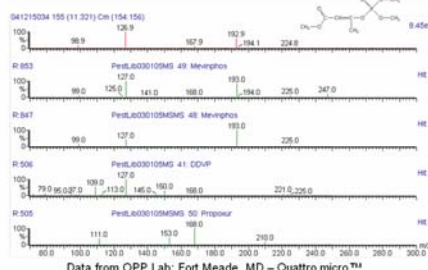
Overview



- LC-MS analysis performed on a water sample
- Resulting chromatograms processed to screen for deleterious compounds
- Full scan mass spectra searched using our Library System
- A good match (>80% probability) indicates a TIC (tentatively identified compound)
- Compound can be further confirmed via MS/MS using our Library System and set conditions

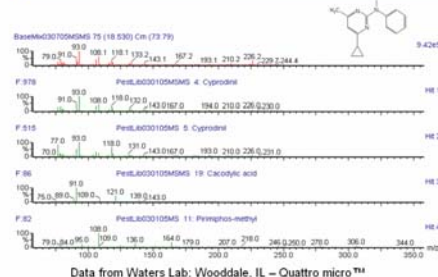
LC-MS Library System

Step 1: Screening and Tentative Identification by MS



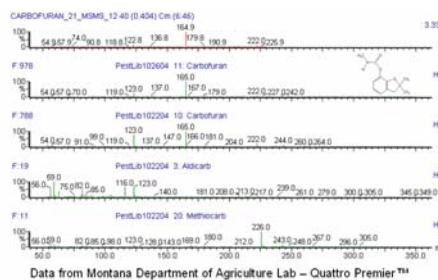
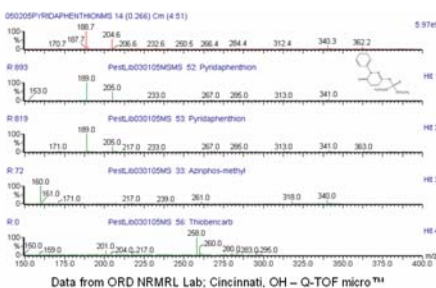
LC-MS Library System

Step 2: Further Confirmation by MS/MS



Conclusions

- LC-MS Library System applicable to screen for selected harmful organic compounds in clean, environmental water samples
 - Drinking water
 - Well water
 - Clean surface waters
- Ability to transfer LC-MS libraries between environmental and agricultural labs
- Qualitative and semi-quantitative approaches
- No extraction, minimal sample preparation



Current Collaborators

- US EPA Office of Research and Development (ORD) NMRL Cincinnati, OH
 - Marc Mills
 - Bryan Boulanger
- US EPA Office of Pesticide Programs (OPP) Fort, Meade, MD
 - Adrian Burns
 - Paul Golden
 - Patricia Schermerhorn
 - Diane Rains
- Waters Corporation Milford, MA
 - Joe Romano
 - Wooddale, IL
 - Harold Johnson
- Montana Department of Agriculture
 - Angie Schaner



Future Collaborators

- US EPA Office of Research and Development (ORD) NERL Las Vegas, NV
 - Christian Daughton
- State of Oregon Department of Environmental Quality
 - Ted Haigh
- Office of Indiana State Chemist
 - Jeff Hardy
- State of Florida Chemical Residue Laboratory
 - Walter Hammack
- Minnesota Department of Agriculture
 - Phillip Hansen
- Minnesota Department of Public Health
 - Paul Swedenborg

Interested?? Contact us...

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Waters



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